Gap analysis for an adiabatic approach to the Exact Cover problem

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Abstract: This paper studies the Exact Cover problem through the lens of Adiabatic Quantum Computation. It contains an introduction to the way an adiabatic computation solves a satisfiability problem, as well as further discussion on how finding and exploiting symmetries hidden in the clauses of the problem can create a speed-up over the conventional procedure.

I. INTRODUCTION

The inception of Quantum computation dates back to the 1980s, but not until recently has the technology been available to build reliable quantum computers. An adiabatic quantum computation is characterized by being a procedure that not rely on the standard gate model. This methodology, however, is equally universal. Only a relative polynomial overhead is needed to encode the adiabatic method to the gate model. The adiabatic theorem assures that starting from an easy to prepare initial state, a slow enough evolution leads to the ground state of the Hamiltonian where the answer has been codified.

This particular way of computing has become the main tool used when solving optimization problems, one of which is the Exact Cover problem. The difficulty when solving this problem appears as its minimum gap energy vanishes at a high number of qubits, therefore, a way to improve the effectiveness of this adiabatic method is coming up with strategies that widen said gap. One such way of improving the gap energy is by exploiting possible hidden structures in the Exact Cover problem, and using them on the Hamiltonian to gain an advantage.

II. ADIABATIC QUANTUM COMPUTING

An Adiabatic Quantum Computation is governed by two k-local Hamiltonians. The initial Hamiltonian, defined as H_0, has a product ground state, and is characterized by being easy to prepare. The Problem Hamiltonian, defined as H_P, is where the problem is encoded and constitutes the output state of the Hamiltonian [1]. The two before-mentioned Hamiltonians are linked by the adiabatic parameter, also known as *schedule*, s. Establishing the schedule as $s(t) : [0, t_f] \to [0, 1]$, the form the Adiabatic Hamiltonian takes is:

$$H(s(t)) = (1 - s(t)) H_0 + s(t) H_P. \tag{1}$$

Starting the system from the ground state of H_0, varying the adiabatic parameter s sufficiently slowly, the adiabatic theorem [2] proves that the final state of the Adiabatic Hamiltonian $H(s(t))$ will be approximately kept in a ground state. This final state after the evolution will then be the ground state of the Problem Hamiltonian H_P.

The time needed to perform the adiabatic sweep and still recover the ground state at the end of the evolution, depends on the energy difference between the ground state and the first excited state, referred to as the *gap energy*. Should this gap become exponentially small, perturbations during the evolution might excite the initial state to one with higher energy, and the output would no longer remain in a ground state [2]. Defining the minimum energy gap as:

$$\Delta \equiv \min_{s\in[0,1]} \Delta(s) = \min_{s\in[0,1]} \epsilon_1(s) - \epsilon_0(s), \tag{2}$$

the time, t_f, needed to compute a problem using an adiabatic approach scales with this quantity. The version of the adiabatic theorem by Elgart *et al.* [3] yields a scaling of t_f with the inverse of the minimum gap squared,

$$t_f \geq \frac{K}{\Delta^2}, \tag{3}$$

up to logarithmic corrections, with a positive constant K in units of energy. For NP-Complete problems, this gap energy, Eq.(2), vanishes exponentially, hence the difficulty of solving this types of problems using an adiabatic method. But should there exist a way to optimize that minimum gap, the time needed to perform a computation with the same precision would decrease.

III. EXACT COVER PROBLEM

The Exact Cover problem is a type of satisfiability problem, and is classified as one of Karp's 21 NP-complete problems [4]. The Exact Cover problem is characterized by only having one bit string that satisfies all its clauses. Considering a number of n boolean variables, that can take the value of either 1 or 0, the Exact Cover problem is defined by a set of clauses, each consisting of 3 of the before mentioned bits, labeled as i, j and k, that must satisfy the constraint $z_i + z_j + z_k = 1$. A set of clauses that leads to a single set of $\{z_1, z_2, z_3, ..., z_n\}$ that fulfill all of them at the same time is called an Exact Cover problem. Checking all possible iterations of a $\{z_1, z_2, z_3, ..., z_n\}$ set to determine if one matches all the clauses of the problem is exponentially hard to solve.

IV. ADIABATIC IMPLEMENTATION OF THE EXACT COVER PROBLEM

In order to solve an Exact Cover problem using the tools provided by the adiabatic principle, from the basic Adiabatic Hamiltonian in Eq.(1), a suitable Problem Hamiltonian H_P that codifies the clauses of the problem, as well as the initial Hamiltonian H_0 are to be constructed. To highlight the effect the algorithm has on the optimization, the schedule variable is kept linear, following $s(t) = \frac{t}{t_f} \to t : [0, t_f]$.

The adiabatic theorem does not state the form of the initial Hamiltonian apart from having an easy to prepare product ground state. The initial Hamiltonian H_0 can be taken either as a sum over σ^x [5] or as the magnetic field in the x direction [6]. In this instance, the initial Hamiltonian takes the form of the latter,

$$H_0 = \sum_{i=1}^{n} \frac{d_i}{2} \left(1 - \sigma_i^x\right), \tag{4}$$

where the parameter d_i is defined as the number of clauses where each qubit i makes an appearance. This initial Hamiltonian has been chosen for ease of interpretation. The addition of the number of appearances of each qubit in the instance translates in an energy evolution over the adiabatic sweep with a more intuitive shape. For an actual computation using a real quantum device, the initial Hamiltonian, therefore the initial state, could be adapted to the one the device finds easier to prepare.

To map the solution of an Exact Cover instance to the Problem Hamiltonian, H_P, a series of Hamiltonians associated to each clause of the problem, H_C, must be defined. By introducing the operator Z as

$$Z \equiv \frac{\mathbb{1} - \sigma^z}{2}, \tag{5}$$

that returns the value 0 or 1 depending on the value of σ^z, the Hamiltonian associated to a clause C_{ijk} is defined as:

$$H_{C_{ijk}} = \left(Z_i + Z_j + Z_k - 1\right)^2, \tag{6}$$

with indexes $\{i, j, k\}$ reflecting the three different qubits in the given clause C_{ijk}. The eigenstates that satisfy the ground state of this Hamiltonian correspond to the solution that satisfies the clause, all other combinations, on the other hand, reach higher energies, since the quadratic nature of Eq.(6) penalizes the non-fulfilling combinations with a positive energy. This operator Z is also introduced by Farhi *et al.* [7] although the final clause Hamiltonian is written in a different way.

Since an Exact Cover instance is governed by the fulfillment of all clauses, the Problem Hamiltonian H_P can be then constructed in the following way:

$$H_P = \sum_{C \in instance} H_C. \tag{7}$$

The ground state of the Problem Hamiltonian is still the eigenstate with zero eigenvalue, as all the clauses contribute with a positive energy in the event of not being satisfied.

A. Optimization Algorithm

The Exact Cover problem requires a single solution to be found, this is a hint that a certain structure is necessary to vanish all the other possible states. Exploiting this structure is how a quantum computer can gain a computational edge over a classical machine. The number of clauses needed to cover the space of possibilities increases with the number of qubits in the system. This means that with a high probability, there is bound to be a high repetition of the same qubits in the clauses. This fact leads to the conclusion that some clauses might be more important regarding the difficulty of the problem. Indeed, the hardest clause is the one that finally closes the system and makes it converge on the unique solution.

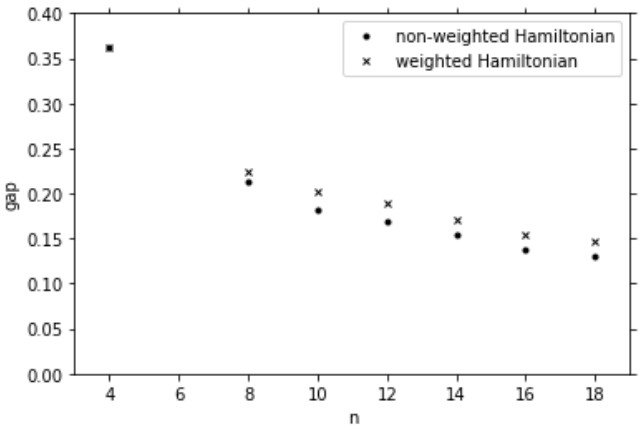

FIG. 1: Average minimum gap of the weighted and non-weighted Hamiltonians as a function of the number of qubits. The average is done over 200 different instances. The gap gain starts small, as with less clauses the structure is harder to be exploited. With an increasing number of qubits the minimum gap energy grows; reaching, and slightly surpassing, 10%.

The importance of a clause in a particular instance is marked by the repetition of its members throughout all other clauses. Using the variable d_i introduced at the creation of the initial Hamiltonian H_0, the number of times the qubit i appears among all clauses, the weight assigned to each clause can be calculated using the equation

$$W_{C_{ijk}} \equiv \left(d_i + d_j + d_k - 3\right), \tag{8}$$

where 3 is subtracted to the sum of the number of appearances of the three qubits in order to achieve the repetition within the other clauses. The better results are achieved if the weights are calculated this way, each clause only seeks repetitions outside of itself.

The weights are then normalized, so that the maximum energy reached by the weighted Hamiltonian remains the same as the non-weighted one. This normalization process is of utmost importance to check the validity of the algorithm, since an unrestrained adding of energy to the Hamiltonian, in the form of non normalized weights, would increase the energy of the first excited state and give a false impression of a wider gap, not provided directly by the algorithm. The clauses of the original Hamiltonian can be considered to have an equal weight of 1, so the sum of all calculated weights should also adhere to the same value. Normalization should then follow:

$$w_C \equiv W_C \frac{n^o clauses}{\sum_{C \in instance} W_C}; \tag{9}$$

so that:

$$\sum_{C \in instance} w_C = n^o clauses. \tag{10}$$

It is easily checked that in the event of maximum energy both Hamiltonians result in the same eigenvalue, since the sum of all weights remains the same and the eigenvalue of the squared sum of operators Z, in both Eq.(6) and Eq.(11), results in the same value in any clause of the instance. An effective way to check if the process

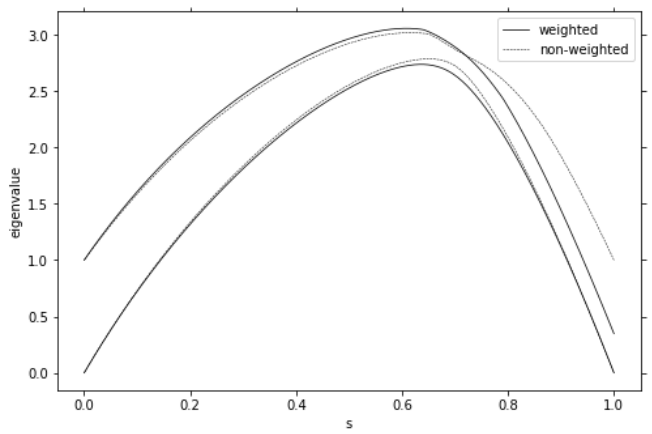

FIG. 2: Comparison of the evolution of the first two eigenvalues during the adiabatic sweep, between a non-weighted and a weighted Hamiltonian for a 10 qubit Exact Cover instance. The behavior is almost exactly identical except for the zone where the gap is reduced to the minimum value, near s 0.7. Even though the gap increases, the maximum energy reached by both Hamiltonians remains the same.

has been successful, not only normalizing the maximum energy of both Hamiltonians, but also the lower energy states, is the comparison of the energy with both the weighted and non-weighted Hamiltonians seen in Fig.(2), that solidifies that the normalization process used is accurate.

Simply adding this weight as a multiplicative term in Eq.(6) results in a weighted Clause Hamiltonian

$$H_{C_{ijk}} = w_{C_{ijk}} \left(Z_i + Z_j + Z_k - 1\right)^2, \tag{11}$$

that can then be summed over in the same way as Eq.(7) for a final Problem Hamiltonian with the same output state for the ground state.

The gain achieved by the algorithm seams to stabilize around 10% judging by the data in Fig.(1). However, for 10 qubits and over the gain starts to slowly increase as the qubits in the system grow in number. This increment reaches over 2% at 18 qubits. This fact is highly non-trivial, as the gap is assumed to always decrease as more qubits are added to the system, but as the clauses for more qubits also increase, the structures that the algorithm uses to speed-up the problem become more robust as well, hinting at a possible gain at larger number of qubits. With that being said, further testing in a higher number of qubits is required to verify this hypothesis.

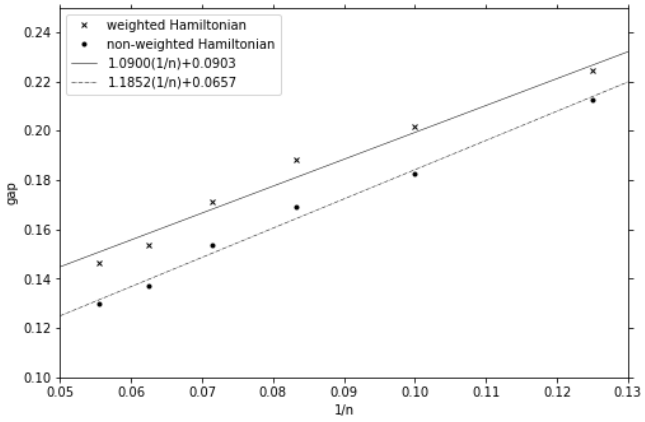

FIG. 3: Average minimum gap of the weighted and non-weighted Hamiltonians as a function of the inverse number of qubits, averaged over 200 different instances. The 4 qubit value is used for the linear regression but is omitted in this representation for clarity. The gap has a clear linear relation with the inverse number of qubits in both cases. The weighted Hamiltonian, however, has a less steep slope; evidence that the algorithm applied provides a better gain in gap energy than just a constant value.

B. Adiabatic simulation of the weighted Hamiltonian

In order to test the gain that the algorithm achieves, a simulation of an actual adiabatic evolution is implemented using the tools provided by the *Qutip* library in the computing language *Python*. The program that outputs this simulation is built following lectures linked to the documentation of said library [8]. For both the original and weighted Hamiltonians, with an equal parameter for the adiabatic sweep in both of them, the probabilities of finding the final state in the ground state are shown

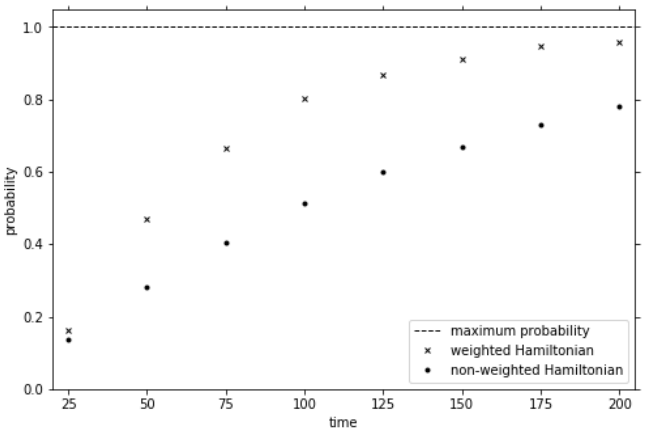

FIG. 4: Probability of finding the ground state of the Adiabatic Hamiltonian as a function of t_f for a non-weighted and a weighted Hamiltonian. Data taken from a simulation of an Exact Cover instance of 14 qubits. As time increases the probability grows in both cases, but the gain is much more significant for the weighted Hamiltonian at every step. In this particular instance, a more satisfying probability is found with a weighted Hamiltonian in half the time spent on the computation.

in Fig.(4). Following the reasoning put forward by Farhi *et al.* [9] the first time shown is the one after achieving a probability of $p = \frac{1}{8}$ of finding the ground state. It can be argued that beyond this probability one can consider the adiabatic evolution to have been successful.

C. Further modifications

The results above show that the algorithm applied heads in the right direction in exploiting possible structures in the Exact Cover problem. However, a better optimization of the time required for the adiabatic sweep may be achieved with some further fine tuning. A more precise control over each qubit might yield even better results. Providing the cancellation needed to achieve the desired ground state of the Problem Hamiltonian is accomplished, a non-trivial characterization of the repetition in the clauses may possibly result in an even wider gap energy.

Another advantage the proposed algorithm provides, is the fact that it acts independently of the variable that governs the adiabatic sweep. For the purpose of this demonstration, the schedule variable grows linearly from 0 to 1. Any process of optimization that is applied to the variable s is perfectly compatible with the above algorithm. Proposing a function $s(t)$, with a smoother behavior where the energy gap reaches the minimum value, is one way to add an extra layer of preciseness to the output state of the Hamiltonian.

To further prove the versatility of this procedure, it could also be improved via a third method. By adding a catalyst Hamiltonian H_s [1] to the Adiabatic Hamiltonian, Eq.(1), in a way that only appears during the intermediate stage of the evolution,

$$H(s) = (1-s)\,H_0 + sH_P + s\,(1-s)\,H_s, \qquad (12)$$

another speedup can be achieved. Even a randomly chosen catalyst Hamiltonian can help [10], but with concrete knowledge of the problem an even better option can be implemented. A *steering Hamiltonian* can be added to the original Adiabatic Hamiltonian in the way depicted in Eq.(12). This Hamiltonian opposes the spin-flip excitations that cause the switch from the ground state to the first excited state during the evolution, in the way proposed in the recent paper by Barış Özgüler *et al.* [11].

V. CONCLUSIONS

- A moderate speed-up has been achieved for the time needed to solve an Exact Cover problem. That means that, as it was proposed, a resemblance of a structure exists in the Exact Cover problem. The symmetry exploited has amplified the minimum gap energy quite a bit, but there is no guarantee that this particular procedure is the limit. A much finer control could yield better results. A further study on the weight space could uncover much finer correlations that could point towards a more exact way to proceed in the weighting of the Hamiltonian.

- This method of optimization is totally non-intrusive to other forms of potential speed-up. This makes it perfectly applicable to any program that solves the Exact Cover problem and is looking for a better performance. Other methods mentioned, ranging from spin steering to controlled alterations to the schedule variable, will only add to the effectiveness of the algorithm.

- The code created to solve the Exact Cover problem is a universal way to solve any of them, provided a set of clauses is given. This means that it could be easily implemented in a universal library for quantum computing, such as QIBO, giving the algorithm a platform from which it could be connected to an actual quantum annealer or a quantum simulator. This fact could give easy access to this problem solving tool to anyone interested in using it.

Code: https://github.com/igres26/exact_cover_gap_analysis

Acknowledgments

Huge thanks to my advisor J. I. Latorre, for guidance and counseling during these 4 months, as well as to all

the members of the Quantic Group for fruitful weekly discussions. Thanks also to my parents and family members for their support.

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